Name: ______________________________

PHYSICS 619 : SPRING SEMESTER 2019

HW #11: Time-dependent Schrodinger Equation

1.) Repeat the same calculation as problem 2 in HW10, but now uses the Generalized Metropolis algorithm, which is the Langevin algorithm with an acceptance/rejection step. Verify that the result you get now is independent of Δt.

2.) The Generalized Metropolis algorithm removed the step-size error by an additional acceptance/rejection step, which adds substantial overhead. To improve on the first-order Langevin algorithm, can you devise a second-order Langevin algorithm to reduce the step-size error dependence to $(\Delta t)^2$? Repeat problem 2 of HW10 using this second-order Langevin algorithm.

3.) Solve the time-dependent Schrodinger equation using the second-order FFT method as described in the lecture note.

   a. Examine the given program and see how the kinetic and potential arrays are first, computed only once. Run the program and see that at dt=0.05, the transmission coefficient is 0.518982 as compared to the exact result of 0.52001.

   b. Out put $|\psi(x)|^2$ at t=10, 15, 20, 25.

   c. Compute $T(E)$ as a function of the initial energy for dt=0.05. Repeat the calculation using the fourth-order Forest-Ruth algorithm. Plot these two results against the exact $T_{ex}(E)$ as given in the lecture note. Plot also $T(E) - T_{ex}(E)$ for these two results in the same graph.